Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bioresmethrin: (5-benzylfuran-3-yl)-methyl 2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate

Tae Ho Kim, Ki-Min Park,* Youngeun Jeon and Jineun Kim*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 660-701, Republic of Korea
Correspondence e-mail: kmpark@gnu.ac.kr, jekim@gnu.ac.kr

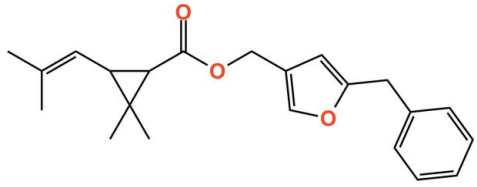
Received 25 September 2012; accepted 27 September 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.096; data-to-parameter ratio = 10.7.

In the title compound, $C_{22}H_{26}O_3$, the dihedral angle between the cyclopropane ring and the plane of the vinyl group is 88.2 (2)°. The dihedral angle between the phenyl and furan rings is 86.09 (8)°. In the crystal, weak intermolecular C—H···π contacts together with very weak C—H···O hydrogen bonds stack the molecules along the a axis.

Related literature

For information on the insecticidal activity of the title compound, see: Hill *et al.* (1993). For a related structure, see: Yang *et al.* (2011).



Experimental

Crystal data

$C_{22}H_{26}O_3$
M_r = 338.43
Monoclinic, $P2_1$
a = 7.8438 (14) Å
b = 11.555 (2) Å
c = 10.9649 (18) Å
β = 108.375 (3)°
V = 943.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 K
0.33 × 0.28 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.992
9877 measured reflections
2458 independent reflections
2156 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.096
S = 1.04
2458 reflections
230 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C1–C6 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O3^{i}	0.99	2.71	3.516 (3)	139
C11—H11···Cg^{ii}	0.95	2.63	3.559 (3)	167

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL*.

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2010–0009089).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5266).

References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany..
Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hill, A. S., McAdam, D. P., Edward, S. L. & Skerritt, J. H. (1993). *J. Agric. Food Chem.* **41**, 2011–2018.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, H., Kim, T. H., Park, K.-M. & Kim, J. (2011). *Acta Cryst.* E**67**, o1275.

supplementary materials

Acta Cryst. (2012). E**68**, o3060 [doi:10.1107/S1600536812040767]

Bioresmethrin: (5-benzylfuran-3-yl)methyl 2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate

Tae Ho Kim, Ki-Min Park, Youngeun Jeon and Jineun Kim

Comment

Bioresmethrin (systematic name: 5-benzyl-3-furylmethyl- 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate), is a synthetic pyrethroid with high insecticidal activity aganist a wide range of insect pests (Hill *et al.*, 1993). However its crystal structure has not yet been reported.

In the title compound (Scheme 1, Fig. 1), the dihedral angle between the cyclopropane ring plane and the vinyl group plane is 88.2 (2)°. The dihedral angle between the benzene and furan ring planes in the benzylfuranyl group is 86.09 (8)°. All bond lengths and bond angles are normal and comparable to those observed in a similar crystal structure (Yang *et al.*, 2011).

In the crystal structure (Fig. 2) weak intermolecular C—H···π interactions [C11···*Cg*^{ii} 3.559 (4) Å. *Cg* is the centroid of the C1—C6 ring. (Symmetry codes: (ii) *x* - 1, *y*, *z*) are found together with very weak C7–H7A···O3 hydrogen bonds, Table 1, stack the molecules along *a*. These intermolecular interactions may contribute to the stabilization of the packing.

Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_2Cl_2 gave single crystals suitable for X-ray analysis.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 1.00 Å, U_{iso} = 1.2U_{eq}(C) for methine C—H, d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for Csp^2—H and d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for CH_3 groups. In the absence of significant anomalous scattering effects, Friedel pairs were merged. Because of this the absolute configuration of the title compound could not be reliably determined from the crystallographic data but has been suggested to be 5-benzyl-3-furylmethyl (1*R*,3*R*)- 2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate from information provided by the manufacturers (the Dr. Ehrenstorfer GmbH Company). However, this cannot be confirmed by the present crystallographic determination.

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

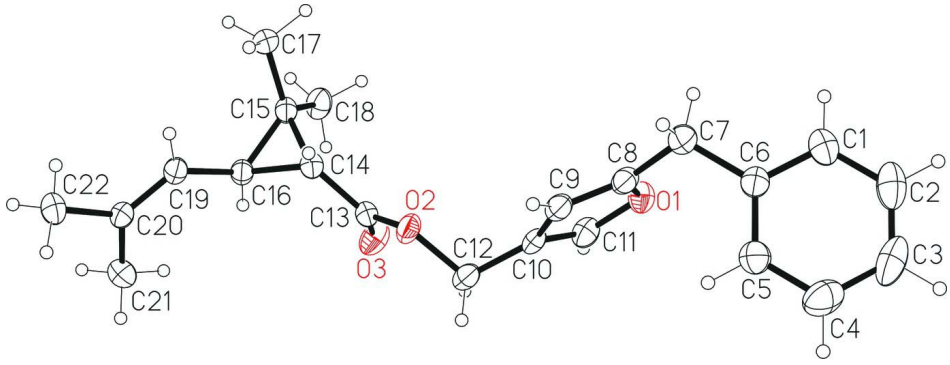


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

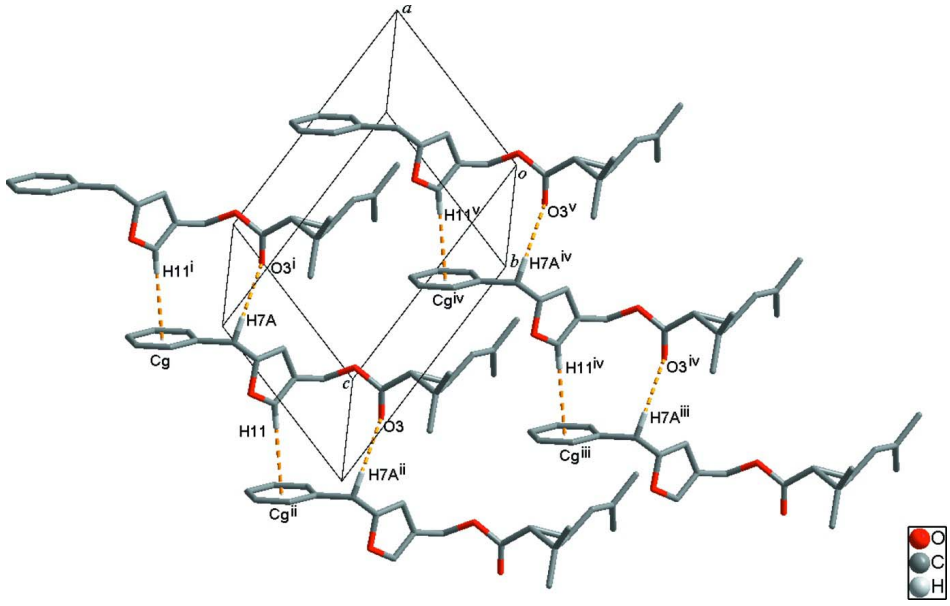


Figure 2

Crystal packing of the title compound with weak intermolecular C—H···π and C–H···O interactions shown as dashed lines. H atoms not involved in intermolecular interactions have been omitted for clarity. (Symmetry codes: (i) $x + 1, y, z$; (ii) $x - 1, y, z$; (iii) $x - 2, y, z - 1$; (iv) $x - 1, y, z - 1$; (v) $x, y, z - 1$.

(5-Benzylfuran-3-yl)methyl 2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate

Crystal data

$C_{22}H_{26}O_3$
$M_r = 338.43$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.8438$ (14) Å
$b = 11.555$ (2) Å
$c = 10.9649$ (18) Å
$\beta = 108.375$ (3)°
$V = 943.2$ (3) Å^3
$Z = 2$
$F(000) = 364$
$D_x = 1.192$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2685 reflections
$\theta = 2.6$–26.3°
$\mu = 0.08$ mm^{-1}
$T = 173$ K
Plate, colourless
0.33 × 0.28 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.992

9877 measured reflections
2458 independent reflections
2156 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −10→10
k = −15→15
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.096
S = 1.04
2458 reflections
230 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 0.1943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6817 (2)	−0.05992 (14)	1.05641 (15)	0.0323 (4)
O2	0.2777 (2)	0.11355 (14)	0.72431 (15)	0.0326 (4)
O3	0.0111 (2)	0.09696 (17)	0.75770 (16)	0.0393 (4)
C1	1.1967 (3)	−0.1520 (2)	1.1670 (3)	0.0378 (6)
H1	1.1775	−0.2312	1.1430	0.045*
C2	1.3371 (4)	−0.1216 (3)	1.2738 (3)	0.0491 (7)
H2	1.4143	−0.1797	1.3230	0.059*
C3	1.3657 (4)	−0.0084 (3)	1.3093 (3)	0.0531 (8)
H3	1.4630	0.0121	1.3830	0.064*
C4	1.2540 (4)	0.0764 (3)	1.2387 (3)	0.0499 (7)
H4	1.2731	0.1552	1.2642	0.060*
C5	1.1138 (3)	0.0463 (2)	1.1306 (3)	0.0363 (6)
H5	1.0381	0.1048	1.0810	0.044*
C6	1.0830 (3)	−0.0685 (2)	1.0940 (2)	0.0286 (5)
C7	0.9302 (3)	−0.1018 (2)	0.9759 (2)	0.0354 (5)
H7A	0.9666	−0.0862	0.8989	0.042*
H7B	0.9087	−0.1860	0.9787	0.042*

C8	0.7591 (3)	−0.03974 (19)	0.9623 (2)	0.0281 (5)
C9	0.6617 (3)	0.03791 (19)	0.8776 (2)	0.0280 (5)
H9	0.6877	0.0674	0.8045	0.034*
C10	0.5105 (3)	0.06772 (19)	0.9187 (2)	0.0274 (5)
C11	0.5305 (3)	0.0060 (2)	1.0258 (2)	0.0320 (5)
H11	0.4492	0.0080	1.0742	0.038*
C12	0.3638 (3)	0.1493 (2)	0.8562 (2)	0.0365 (6)
H12A	0.2748	0.1501	0.9032	0.044*
H12B	0.4128	0.2284	0.8581	0.044*
C13	0.1008 (3)	0.08949 (18)	0.6877 (2)	0.0259 (4)
C14	0.0392 (3)	0.05617 (17)	0.5514 (2)	0.0240 (4)
H14	0.1309	0.0644	0.5059	0.029*
C15	−0.1023 (3)	−0.03703 (18)	0.4976 (2)	0.0255 (4)
C16	−0.1542 (3)	0.08798 (18)	0.4709 (2)	0.0244 (4)
H16	−0.2295	0.1201	0.5214	0.029*
C17	−0.0750 (3)	−0.1108 (2)	0.3920 (2)	0.0316 (5)
H17A	−0.0064	−0.1802	0.4294	0.047*
H17B	−0.0087	−0.0666	0.3454	0.047*
H17C	−0.1920	−0.1337	0.3325	0.047*
C18	−0.1790 (3)	−0.1031 (2)	0.5866 (2)	0.0347 (5)
H18A	−0.2054	−0.0493	0.6474	0.052*
H18B	−0.0916	−0.1608	0.6340	0.052*
H18C	−0.2899	−0.1420	0.5363	0.052*
C19	−0.1846 (3)	0.14189 (19)	0.3437 (2)	0.0267 (4)
H19	−0.1285	0.1057	0.2885	0.032*
C20	−0.2821 (3)	0.23548 (19)	0.2982 (2)	0.0276 (5)
C21	−0.3813 (4)	0.3044 (2)	0.3695 (3)	0.0390 (6)
H21A	−0.3744	0.2650	0.4501	0.058*
H21B	−0.5075	0.3120	0.3167	0.058*
H21C	−0.3273	0.3815	0.3885	0.058*
C22	−0.2964 (4)	0.2819 (2)	0.1675 (2)	0.0387 (6)
H22A	−0.2335	0.2299	0.1254	0.058*
H22B	−0.2417	0.3590	0.1762	0.058*
H22C	−0.4232	0.2871	0.1156	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0341 (8)	0.0369 (9)	0.0243 (9)	0.0015 (7)	0.0069 (7)	0.0039 (7)
O2	0.0254 (8)	0.0411 (9)	0.0249 (9)	0.0036 (7)	−0.0015 (7)	−0.0062 (7)
O3	0.0382 (9)	0.0543 (11)	0.0258 (9)	−0.0059 (8)	0.0110 (8)	−0.0055 (8)
C1	0.0355 (13)	0.0412 (13)	0.0361 (15)	0.0070 (11)	0.0105 (12)	0.0076 (11)
C2	0.0380 (15)	0.073 (2)	0.0338 (16)	0.0106 (14)	0.0083 (12)	0.0147 (15)
C3	0.0280 (13)	0.094 (3)	0.0340 (17)	−0.0070 (15)	0.0048 (12)	−0.0053 (16)
C4	0.0377 (14)	0.0526 (17)	0.0597 (19)	−0.0127 (13)	0.0159 (14)	−0.0167 (15)
C5	0.0314 (12)	0.0364 (12)	0.0398 (15)	0.0012 (10)	0.0090 (11)	−0.0013 (11)
C6	0.0264 (10)	0.0353 (11)	0.0256 (12)	0.0022 (9)	0.0105 (9)	−0.0010 (10)
C7	0.0353 (12)	0.0376 (12)	0.0296 (13)	0.0068 (10)	0.0051 (10)	−0.0053 (10)
C8	0.0282 (11)	0.0307 (11)	0.0235 (12)	−0.0021 (9)	0.0054 (9)	−0.0049 (9)
C9	0.0298 (11)	0.0297 (11)	0.0223 (12)	−0.0029 (9)	0.0051 (9)	−0.0036 (9)

C10	0.0248 (10)	0.0294 (11)	0.0222 (12)	−0.0033 (8)	−0.0008 (9)	−0.0067 (9)
C11	0.0267 (11)	0.0408 (13)	0.0279 (13)	−0.0030 (9)	0.0079 (10)	−0.0036 (10)
C12	0.0348 (13)	0.0372 (13)	0.0297 (14)	0.0040 (10)	−0.0011 (11)	−0.0121 (11)
C13	0.0269 (10)	0.0230 (9)	0.0245 (11)	0.0024 (8)	0.0034 (9)	0.0028 (9)
C14	0.0231 (10)	0.0260 (10)	0.0226 (11)	0.0016 (8)	0.0066 (9)	0.0022 (8)
C15	0.0255 (10)	0.0257 (10)	0.0223 (11)	0.0012 (8)	0.0032 (9)	0.0024 (9)
C16	0.0239 (10)	0.0267 (10)	0.0216 (11)	0.0026 (8)	0.0056 (8)	0.0007 (9)
C17	0.0377 (13)	0.0253 (10)	0.0271 (13)	0.0009 (9)	0.0034 (10)	−0.0034 (9)
C18	0.0347 (12)	0.0370 (12)	0.0297 (13)	−0.0079 (10)	0.0064 (10)	0.0055 (10)
C19	0.0275 (10)	0.0291 (10)	0.0216 (11)	0.0023 (8)	0.0051 (9)	0.0002 (9)
C20	0.0271 (11)	0.0265 (10)	0.0240 (12)	−0.0010 (8)	0.0008 (9)	−0.0009 (9)
C21	0.0406 (13)	0.0316 (12)	0.0401 (15)	0.0083 (10)	0.0060 (12)	0.0001 (11)
C22	0.0491 (15)	0.0314 (12)	0.0288 (14)	0.0030 (11)	0.0026 (11)	0.0070 (10)

Geometric parameters (Å, º)

O1—C11	1.360 (3)	C12—H12B	0.9900
O1—C8	1.372 (3)	C13—C14	1.470 (3)
O2—C13	1.346 (3)	C14—C15	1.525 (3)
O2—C12	1.450 (3)	C14—C16	1.540 (3)
O3—C13	1.197 (3)	C14—H14	1.0000
C1—C2	1.377 (4)	C15—C16	1.504 (3)
C1—C6	1.385 (3)	C15—C18	1.505 (3)
C1—H1	0.9500	C15—C17	1.508 (3)
C2—C3	1.363 (5)	C16—C19	1.476 (3)
C2—H2	0.9500	C16—H16	1.0000
C3—C4	1.379 (5)	C17—H17A	0.9800
C3—H3	0.9500	C17—H17B	0.9800
C4—C5	1.383 (4)	C17—H17C	0.9800
C4—H4	0.9500	C18—H18A	0.9800
C5—C6	1.384 (3)	C18—H18B	0.9800
C5—H5	0.9500	C18—H18C	0.9800
C6—C7	1.511 (3)	C19—C20	1.327 (3)
C7—C8	1.486 (3)	C19—H19	0.9500
C7—H7A	0.9900	C20—C21	1.495 (3)
C7—H7B	0.9900	C20—C22	1.501 (3)
C8—C9	1.344 (3)	C21—H21A	0.9800
C9—C10	1.437 (3)	C21—H21B	0.9800
C9—H9	0.9500	C21—H21C	0.9800
C10—C11	1.340 (3)	C22—H22A	0.9800
C10—C12	1.478 (3)	C22—H22B	0.9800
C11—H11	0.9500	C22—H22C	0.9800
C12—H12A	0.9900		

C11—O1—C8	106.11 (18)	C13—C14—C16	117.97 (17)
C13—O2—C12	117.90 (18)	C15—C14—C16	58.78 (13)
C2—C1—C6	120.7 (3)	C13—C14—H14	115.1
C2—C1—H1	119.7	C15—C14—H14	115.1
C6—C1—H1	119.7	C16—C14—H14	115.1
C3—C2—C1	120.2 (3)	C16—C15—C18	118.33 (18)

C3—C2—H2	119.9	C16—C15—C17	119.24 (19)
C1—C2—H2	119.9	C18—C15—C17	113.2 (2)
C2—C3—C4	120.2 (3)	C16—C15—C14	61.09 (14)
C2—C3—H3	119.9	C18—C15—C14	119.90 (19)
C4—C3—H3	119.9	C17—C15—C14	115.70 (18)
C3—C4—C5	119.7 (3)	C19—C16—C15	122.87 (18)
C3—C4—H4	120.2	C19—C16—C14	118.61 (17)
C5—C4—H4	120.2	C15—C16—C14	60.13 (14)
C4—C5—C6	120.5 (3)	C19—C16—H16	114.8
C4—C5—H5	119.7	C15—C16—H16	114.8
C6—C5—H5	119.7	C14—C16—H16	114.8
C5—C6—C1	118.6 (2)	C15—C17—H17A	109.5
C5—C6—C7	120.7 (2)	C15—C17—H17B	109.5
C1—C6—C7	120.7 (2)	H17A—C17—H17B	109.5
C8—C7—C6	114.2 (2)	C15—C17—H17C	109.5
C8—C7—H7A	108.7	H17A—C17—H17C	109.5
C6—C7—H7A	108.7	H17B—C17—H17C	109.5
C8—C7—H7B	108.7	C15—C18—H18A	109.5
C6—C7—H7B	108.7	C15—C18—H18B	109.5
H7A—C7—H7B	107.6	H18A—C18—H18B	109.5
C9—C8—O1	110.07 (19)	C15—C18—H18C	109.5
C9—C8—C7	133.7 (2)	H18A—C18—H18C	109.5
O1—C8—C7	116.2 (2)	H18B—C18—H18C	109.5
C8—C9—C10	106.8 (2)	C20—C19—C16	127.0 (2)
C8—C9—H9	126.6	C20—C19—H19	116.5
C10—C9—H9	126.6	C16—C19—H19	116.5
C11—C10—C9	105.50 (19)	C19—C20—C21	124.8 (2)
C11—C10—C12	127.2 (2)	C19—C20—C22	120.7 (2)
C9—C10—C12	127.3 (2)	C21—C20—C22	114.5 (2)
C10—C11—O1	111.5 (2)	C20—C21—H21A	109.5
C10—C11—H11	124.2	C20—C21—H21B	109.5
O1—C11—H11	124.2	H21A—C21—H21B	109.5
O2—C12—C10	109.31 (18)	C20—C21—H21C	109.5
O2—C12—H12A	109.8	H21A—C21—H21C	109.5
C10—C12—H12A	109.8	H21B—C21—H21C	109.5
O2—C12—H12B	109.8	C20—C22—H22A	109.5
C10—C12—H12B	109.8	C20—C22—H22B	109.5
H12A—C12—H12B	108.3	H22A—C22—H22B	109.5
O3—C13—O2	123.6 (2)	C20—C22—H22C	109.5
O3—C13—C14	126.8 (2)	H22A—C22—H22C	109.5
O2—C13—C14	109.55 (17)	H22B—C22—H22C	109.5
C13—C14—C15	122.92 (18)		

C6—C1—C2—C3	0.2 (4)	C12—O2—C13—O3	0.7 (3)
C1—C2—C3—C4	0.2 (4)	C12—O2—C13—C14	179.52 (18)
C2—C3—C4—C5	−0.8 (4)	O3—C13—C14—C15	−37.8 (3)
C3—C4—C5—C6	1.1 (4)	O2—C13—C14—C15	143.42 (19)
C4—C5—C6—C1	−0.8 (4)	O3—C13—C14—C16	31.4 (3)
C4—C5—C6—C7	−180.0 (2)	O2—C13—C14—C16	−147.39 (18)

C2—C1—C6—C5	0.2 (3)	C13—C14—C15—C16	105.1 (2)
C2—C1—C6—C7	179.3 (2)	C13—C14—C15—C18	−2.8 (3)
C5—C6—C7—C8	−43.0 (3)	C16—C14—C15—C18	−107.9 (2)
C1—C6—C7—C8	137.8 (2)	C13—C14—C15—C17	−144.2 (2)
C11—O1—C8—C9	1.3 (2)	C16—C14—C15—C17	110.7 (2)
C11—O1—C8—C7	179.2 (2)	C18—C15—C16—C19	−142.9 (2)
C6—C7—C8—C9	113.6 (3)	C17—C15—C16—C19	1.7 (3)
C6—C7—C8—O1	−63.7 (3)	C14—C15—C16—C19	106.6 (2)
O1—C8—C9—C10	−1.1 (2)	C18—C15—C16—C14	110.4 (2)
C7—C8—C9—C10	−178.5 (2)	C17—C15—C16—C14	−105.0 (2)
C8—C9—C10—C11	0.5 (2)	C13—C14—C16—C19	133.0 (2)
C8—C9—C10—C12	−179.5 (2)	C15—C14—C16—C19	−113.6 (2)
C9—C10—C11—O1	0.3 (2)	C13—C14—C16—C15	−113.4 (2)
C12—C10—C11—O1	−179.7 (2)	C15—C16—C19—C20	156.9 (2)
C8—O1—C11—C10	−1.0 (3)	C14—C16—C19—C20	−131.9 (2)
C13—O2—C12—C10	121.1 (2)	C16—C19—C20—C21	−0.2 (4)
C11—C10—C12—O2	−123.2 (2)	C16—C19—C20—C22	178.4 (2)
C9—C10—C12—O2	56.8 (3)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O3^{i}	0.99	2.71	3.516 (3)	139
C11—H11···*Cg*^{ii}	0.95	2.63	3.559 (3)	167

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*.